Segregation of Network Modifiers in Borosilicate Glasses

Insights from a New Transferable Potential

Wang, Mengyi; Smedskjær, Morten Mattrup; Mauro, John C.; Sant, Gaurav; Bauchy, Mathieu

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

Segregation of Network Modifiers in Borosilicate Glasses: Insights from a New Transferable Potential

Mengyi Wang[1], Morten M. Smedskjaer[2], John C. Mauro[3], Gaurav Sant[1], Mathieu Bauchy[1]

[1]Civil and Environmental Engineering Department, University of California, Los Angeles, Los Angeles, CA, United States

[2]Aalborg University, Aalborg, Denmark

[3]Corning Incorporated, Corning, NY, USA

The existence of network modifying (alkali or alkaline-earth) atoms' segregation or clustering inside silicate glasses remains controversial. Such heterogeneity could play a crucial role in controlling mascroscopic properties, including crystallization propensity, fracture, or dissolution. Here, based on molecular dynamics simulations, we report the existence of such clustering in borosilicate glasses. First, a novel inter-atomic potential was developed for modified borosilicate glasses. This new potential is found to offer an excellent transferability, as, with constant parameters, it correctly predicts the coordination number of boron atoms and the density of the glass over a wide range of Si/B ratios, from silicate to borate glasses. Predicted structure factors are also found to be in good agreement with available experimental data. Second, the simulated structures are analyzed to assess the heterogeneity of the distribution of Ca and Na atoms inside a series of borosilicate glasses. We observe a strong propensity for network modifier clustering, both for Ca and Na atoms. In turn, boron atoms are shown to enhance the homogeneity of the network. The origin of this trend is discussed.

KEYWORDS: Molecular dynamics, Borosilicate, Heterogeneity, Structure, Potential parametrization.